

Science & Technology

REVIEW



Transforming **DESIGN**



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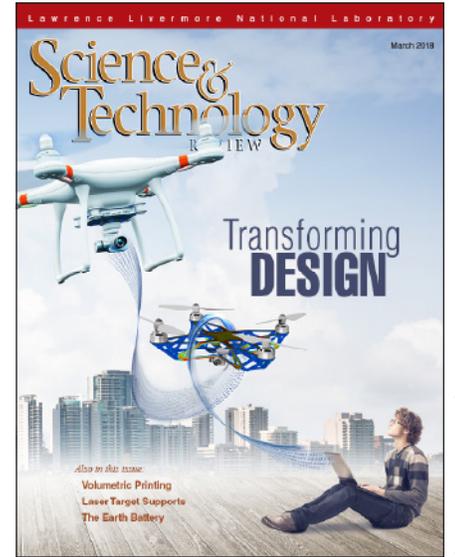
Volumetric Printing

Laser Target Supports

The Earth Battery

About the Cover

Additive manufacturing (AM) technologies allow extreme levels of control over shape and material composition at scales down to nanometers. Livermore's Center for Design Optimization is creating a comprehensive computing environment where Laboratory engineers can take full advantage of AM. One aspect is design optimization, where designs are created automatically by sophisticated numerical algorithms. As the article beginning on p. 4 describes, a three-year effort is under way to develop a software package called Livermore Design Optimization (LiDO). LiDO will help realize the tremendous potential of AM and launch a true revolution in design. The cover depicts an actual drone chassis designed with LiDO hypothetically transforming into a real drone.



Cover design: Mary J. Gines

About S&TR

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3893. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the Web at str.llnl.gov.

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Contents

S&TR Staff

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Ken Chinn

PUBLICATION EDITOR

Paul Kotta

WRITERS

Holly Auten, Lauren Casonhua,
Arnie Heller, Ben Kennedy,
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ART DIRECTOR

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DESIGNER

Acen Datuin

PROOFREADER

Caryn Meissner

S&TR ONLINE

Lauren Casonhua, Rose Hansen,
Lanie L. Helms, and Pam Davis Williams

PRINT COORDINATOR

Diana Horne

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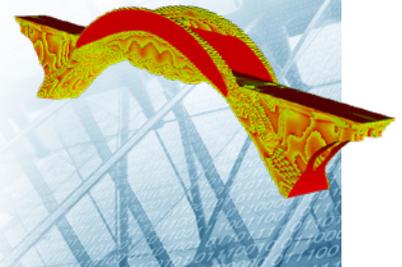
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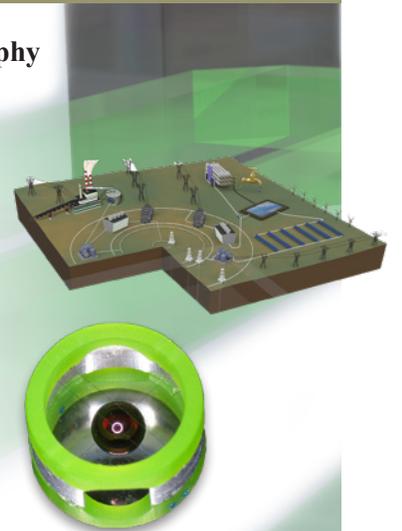
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Predicting Miniaturized Structures' Failure Modes

Lawrence Livermore researchers have adapted theoretical models to predict and demonstrate the failure behavior of miniaturized three-dimensional (3D) lattices, seen in trestle bridges and similar structures. Additive manufacturing—also known as 3D printing—allows researchers to miniaturize these types of structures to considerably smaller length scales than was possible before. Laboratory researchers Mark Messner (now at Argonne National Laboratory) and Holly Carlton published these studies in the May 1, 2017, edition of *Acta Materialia*.

Messner used a newly developed equivalent continuum model to predict failure behavior in lattice structures with different topologies. Understanding the dominant failure mode is critical to using lightweight microtrusses because of the mode's influence on a structure's energy absorption capacity. Messner's method predicts a tradeoff between yield-dominated and catastrophic buckling-dominated failure modes at a critical relative density. This predicted density depends on several modeling assumptions that are strongly influenced by the manufacturing process.

To experimentally investigate deformation in lattice structures, Carlton coupled quasistatic compression tests with in situ tomography at Lawrence Berkeley National Laboratory's Advanced Light Source. These experiments on miniaturized 3D-printed unit cell lattice structures captured real-time deformation, specifically showing a transition in failure mode from catastrophic buckling to yielding at a low relative density, thus validating Messner's model predictions. These findings have implications for how scientists and engineers design and fabricate architected structures for future applications.

Contact: Holly Carlton (925) 422-2765 (carlton4@llnl.gov).

"Heart-on-a-Chip" Unveiled

Livermore researchers have measured the effects of drug exposure on heart tissue using "heart-on-a-chip" technology—an engineered chip that models the human heart. This research, published in the May 21, 2017, edition of the journal *Lab on a Chip*, seeks to shorten new-drug trials and ensure that potentially lifesaving drugs are safe and effective.

The paper describes the successful recording of both electrical signals and cellular beating from normal heart cells grown on a Livermore-developed multielectrode array. (See rendering above.) This design is the first capable of simultaneously mapping both the electrophysiology and contraction frequency of the cells. The tissue was exposed to the stimulant norepinephrine, resulting in



increases in the cells' electrical signal and beating, replicating what happens in the human body. The researchers state that the chip can benefit pharmaceutical companies not only by serving as an early alert for cardiac problems caused by a drug but also by providing experimental information about drug functions so that better compounds can be designed. The technology may also reduce the need for human and animal testing.

The heart-on-a-chip uses cultured human cardiac cells, which naturally and spontaneously grow to form a layer of heart tissue that begins to beat after only two days in culture. Over time, the researchers demonstrated that the platform could measure heart tissue growth, electrophysiology, and heartbeat simultaneously and in real time. The Laboratory Directed Research and Development Program funded the project as part of its iCHIP (in vitro chip-based human investigational platform) effort. Livermore collaborated with Harvard Medical School in the research.

Contact: Elizabeth Wheeler (925) 423-6245 (wheeler16@llnl.gov).

Peering at the Crystal Structure of Lithium

Lawrence Livermore researchers recently proposed a technique to obtain structural information about lithium under conditions at which traditional crystallographic methods are insufficient, possibly solving a decades-long puzzle. Although lithium is considered a typical, simple metal, its crystal structure at ambient pressure and low temperature has remained unknown.

In a paper appearing in the May 23, 2017, edition of *Proceedings of the National Academy of Sciences*, the researchers describe measuring oscillations of lithium's crystal magnetic moment in an external magnetic field. The team performed theoretical analysis showing the spectrum of oscillation resonances to be quite distinctive for different lithium structures. A comparison with previous experimental data indicates that the low-temperature phase of lithium is incompatible with the previously attributed structure of nine hexagonal stacking layers.

Lithium and its compounds have several industrial applications, including heat-resistant glass and ceramics, grease lubricants, flux additives for metal production, and lithium-ion batteries—uses that represent more than three-quarters of lithium production. For years, however, scientists have tried to understand lithium's strange behavior and structure. Calculations to determine the lowest energy equilibrium structure require enormous precision. In addition, the element's light atomic mass results in significant dynamics even at low temperature and a relatively weak response to x rays and neutrons—the traditional methods for determining crystal structure. Furthermore, the transition to the low-temperature phase is gradual and breaks the single-crystal structure. This recent breakthrough by Laboratory researchers enables more-precise analysis of lithium.

Contact: Stanimir Bonev (925) 422-4347 (bonev2@llnl.gov).



Giving Engineers Powerful New Design Tools

THIS issue's feature article, beginning on p. 4, focuses on a concerted effort to develop novel design optimization algorithms, methodologies, and software to enable the rapid design of advanced systems, components, and material architectures. With recent breakthroughs in advanced manufacturing—several of which are being enabled by Laboratory researchers—our ability to manufacture complex components and materials has far outpaced our ability to design. Designers, no longer merely inconvenienced by inefficient trial-and-error design, are nearly incapacitated by the vast space of possible designs now afforded by advanced manufacturing technologies. No systematic methods currently exist to explore this vast design space for systems with significant complexity, especially systems of interest to the National Nuclear Security Administration (NNSA), namely, those exhibiting nonlinear, transient, multiscale, and multiphysics phenomena with uncertain behavior.

Although commercial software has been successfully employed to optimize large-scale engineering problems, such software is predominantly limited to simplistic design parameterizations and optimization metrics and assumptions of linear behavior. Academic research solves problems that are more complex but significantly smaller in scale. The engineering community has yet to address the problem of simultaneous optimization over complex design and response spaces in the type of large-scale high-performance computing (HPC) environment that fully leverages the possibilities afforded by today's advanced manufacturing breakthroughs. The novel research effort described in the feature article aims to close this gap and provide solutions to NNSA's critical design problems.

To this end, a team of researchers from Livermore and leading universities is creating a comprehensive design optimization software package called Livermore Design Optimization (LiDO). The team's goal is to fundamentally transform design by using LiDO to suggest radically novel designs that fulfill all the requirements—such as weight, strength, and stiffness—specified by the user. The process of converging to a single design from a set of requirements is often described as inverse design, which, along with optimization, is one of the most compelling frontiers of computational engineering research today.

Complexity in design optimization arises from two sources: design and physics. The complexity of design involves the intricate shapes and material layouts made possible by advanced

manufacturing technology, such as structural composites with intricate morphologies and architectures. Design complexity also refers to the strength, stiffness, and other metrics that an engineer seeks to optimize. Physics complexity comes from the mathematical models used to predict design performance. Such models require the solution of partial differential equations involving complex nonlinearities, transients, multiple scales, multiple physics, and uncertainties. Designers usually iterate through the design space, solving the physics equations using numerical methods. With typical degrees of freedom in design and physics exceeding 1 billion, solutions require efficient algorithms running on HPC systems. However, design iterations are usually guided by the engineer's intuition, with no quantitative way to ensure that the final design will be optimal. LiDO can revolutionize design by allowing engineers to automatically converge to an optimal design, factoring in all constraints and solving problems of unprecedented complexity and scale. More importantly, this novel capability will make possible highly nonintuitive designs that were previously unobtainable.

The past few years have seen remarkable progress in applying additive manufacturing to the Laboratory's core mission of maintaining the nation's nuclear weapons stockpile. For example, as described in the research highlight beginning on p. 12, researchers have invented a method to use light beams to fabricate three-dimensional polymer structures volumetrically and monolithically in a few seconds, rather than building up layer by layer. The Laboratory is also demonstrating additive manufacturing with polymers, metals, ceramics, semiconductors, and novel combinations of materials, creating new opportunities to solve critical national security issues. Additive manufacturing is also enabling advanced batteries; printed biological tissues; and catalytic reactors to convert greenhouse gases into valuable, long-lived products.

Laboratory researchers continue to add powerful new manufacturing tools to their existing toolset to combine novel shapes, internal structures, and physical properties that were impossible to realize in the past but are now limited only by one's imagination. With LiDO on the horizon, I look forward to continued advances that will surely bolster nearly every area of Laboratory research and U.S. industry.

■ Anantha Krishnan is associate director for Engineering.

LEADING A REVOLUTION

*Livermore researchers are creating powerful software
for designing objects previously unobtainable.*

in DESIGN

ADDITIVE manufacturing technologies—often called three-dimensional (3D) printing—represent a revolution in how products are made. Now being adopted by U.S. industry, the approach allows an extreme level of control over shape and material composition at scales down to nanometers, creating the potential to engineer materials with desired structural, thermal, electrical, chemical, and photonic properties in a single package. Novel structures having complex microarchitectures and composed of metals, polymers, and ceramics are being created. In some cases, multiple materials are combined to create “metamaterials” with properties never before possible.

Engineers and computer scientists at Lawrence Livermore are working together to produce new materials with additive manufacturing, drawing on expertise in precision engineering, highly detailed computer modeling and simulations, materials science, and high-performance computing (HPC). The new parts and systems, intended for Livermore’s national security missions, offer greater performance, reduced time to manufacture, less waste, and often lower cost.

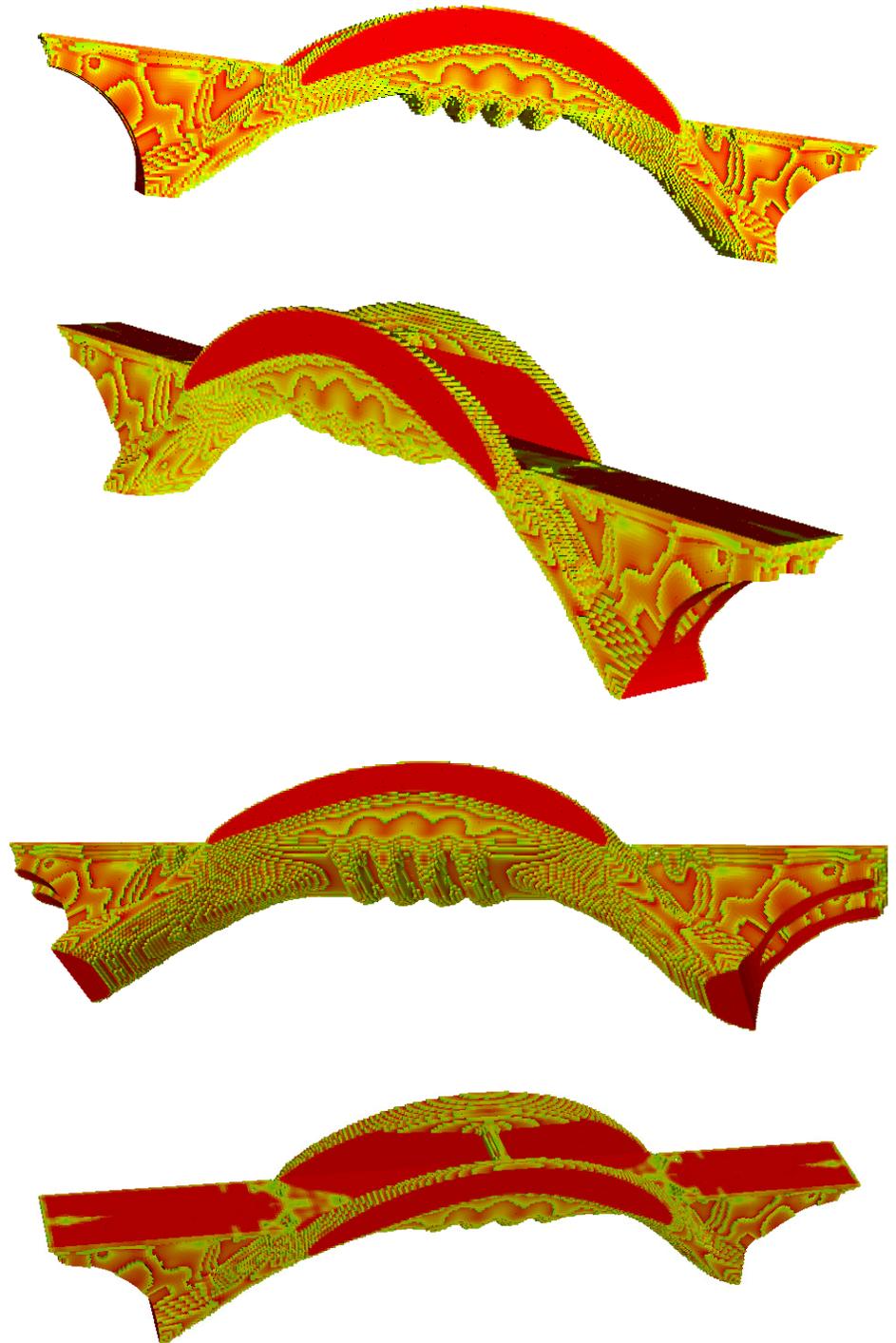
Because additive manufacturing eliminates many previous manufacturing constraints, engineers are beginning to rethink design basics and how to achieve products with greater complexity and

enhanced performance. However, without formal design paradigms that take full advantage of the technique's potential, researchers currently generate designs for additive manufacturing using a costly trial-and-error approach based on conventional design tools such as computer-aided design and computer-aided engineering (CAE) software, guided solely by the engineer's experience and intuition. Such practices all too often result in only incremental improvements to existing designs.

Replacing Trial and Error

Mechanical engineer Dan Tortorelli, who leads the Laboratory's Center for Design Optimization, is working to fundamentally transform how engineers design complex parts and systems to be additively manufactured. Tortorelli says, "Our ability to manufacture exceeds our ability to design. Design has become a bottleneck, in that designing a part for additive manufacturing is sometimes more difficult than actual fabrication." Engineers can face a bewildering number of possible designs when striving for the necessary combination of nonlinear, transient, multiscale, and multiphysics attributes in a part or system. "The opportunity and need to fundamentally transform design is one of the most compelling frontiers in engineering," says Tortorelli. "We want to give engineers the tools to help them rethink what is possible. New shapes with new internal structures that would have been prohibitively costly or even impossible to manufacture only a few years ago are now possible."

Tortorelli states that conventional design methods and computer algorithms are constrained by outdated presumptions about material properties and manufacturing methods and do not take advantage of the modeling and simulation capabilities, data analytics, and algorithms that are common in HPC. As an example he compares a modern-day composite airplane fuselage to a centuries-old wooden ship. Except for modern materials, the designs are strikingly similar. In short, simply using



This projection shows a 60-meter-long bridge designed by Livermore Design Optimization (LiDO) software. The design inputs for LiDO included a "bounding box" to fill with material and a load distribution representing car weight. The design is optimal in that for a given weight, stiffness is the maximum possible. To enhance stiffness, the design features four ribs on the bridge's underside and a cross member between the arches.

additive manufacturing to fabricate products designed with conventional techniques misses the point. Chris Spadaccini, director of Lawrence Livermore's Additive Manufacturing Initiative, adds, "Without a proper HPC-based design framework, engineers risk leaving much manufacturing capability on the table. Control of microarchitecture offers the potential for materials designed with new functionalities and an order-of-magnitude improvement in performance." (See the box on p. 10.)

Leveraging Computation

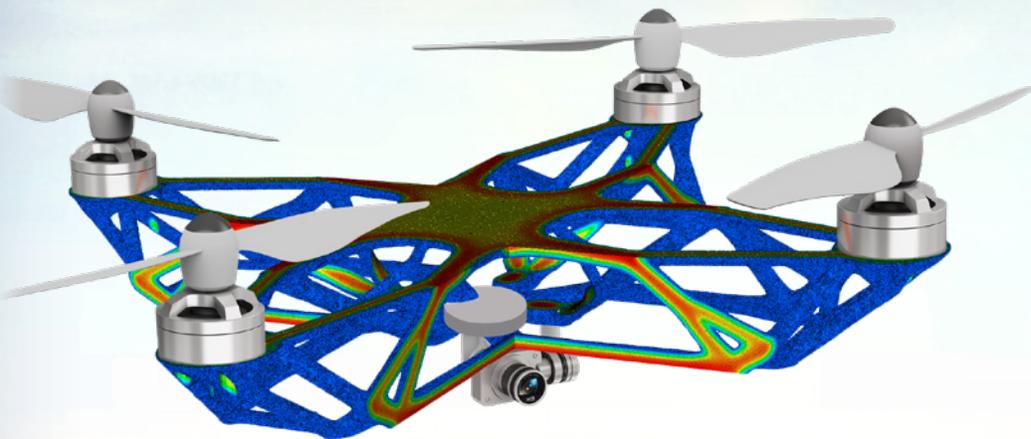
The Center for Design Optimization was established in October 2016 in response to the critical need for a comprehensive computing environment that takes full advantage of additive manufacturing. With funding from the Laboratory Directed Research and Development Program, the center launched a three-year Computational Design Optimization Strategic Initiative led by principal investigators Tortorelli and

computational engineer Daniel White. In this effort, more than a dozen Livermore computer scientists and engineers are leveraging the Laboratory's extensive HPC capabilities to develop an efficient design optimization software package called Livermore Design Optimization (LiDO). Collaborators include researchers from the University of Illinois; Lund University, Sweden; the University of Wisconsin; the University of Texas at Austin; Technical University, Denmark; the International Computing Science Institute, in Berkeley, California; and CAE software firm Autodesk, Inc., based in San Rafael, California.

The team's goal with LiDO is to provide a cohesive design environment where Livermore's rapidly growing additive manufacturing capabilities are seamlessly combined with HPC resources such as codes, algorithms, powerful modeling and simulation tools, data analytics, and some of the world's most powerful

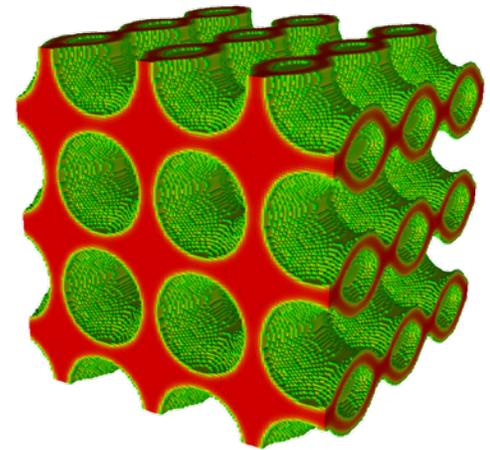
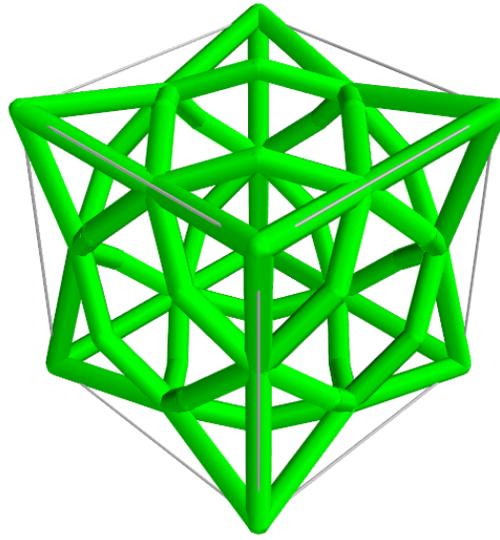
supercomputers. The fully integrated LiDO combines multiple length scales, geometric representations, multiresolution capability, multiphysics, and uncertainty factors for optimizing designs characterized by transient and nonlinear phenomena. LiDO systematically traverses the design space to obtain the shapes and microarchitectures that best meet the requirements specified by the user.

Rob Sharpe, deputy associate director for research and development in Livermore's Engineering Directorate, tells how managers in the directorate began to think about the need to transform design work as colleagues began investigating, adopting, and inventing additive manufacturing processes as part of Engineering's Advanced Materials and Manufacturing Initiative. "We began to explore the possibility of first describing the desired functions of a new part—such as the size and properties—and then turning the computer loose to arrive at the best design."



This design for a drone chassis with four rotors accommodates two different loads—the upward force of the rotors and the downward pull of gravity, especially on the camera and batteries. Design optimization with LiDO software required Livermore's Vulcan supercomputer and used 100 million mesh elements—well beyond the capability of commercial software.

Tortorelli says, “We want to enable the design of systems that were previously unobtainable, unthinkable, and unimaginable.” By providing the best design tools, the LiDO development team anticipates nonintuitive, high-performing designs for Laboratory missions in national and global security, lasers, and energy. The code takes into account a host of objectives such as weight, volume, and manufacturability. Ensuring manufacturability enables an engineer to consider only those designs that are readily buildable. Collaborating researchers at the University of Wisconsin are working to quantify manufacturing uncertainty and ensure robust designs that are resistant to defects.



Two examples of unit cells, the basic component of an additively manufactured part or system, are shown. Both are designed for maximum stiffness and are of arbitrary dimensions. Aggregates of these cells can form microtrusses to serve as building blocks for much larger structures, ranging from bridges to antennas.

Liberating Engineers

Sharpe points out that Livermore engineers are often charged with design tasks that go far beyond intuition because of their scale and complexity. An engineer can confidently understand the forces that a static object such as a solid bridge must withstand and test the object virtually for its response to these forces. However, intuition is severely limited when thinking about structures that operate in the nonlinear regime or when many different physics are involved. For example, a part may have to take into account a combination of structural, thermal, optical, and electrical phenomena, ranging from the speed of sound to the speed of light. A part may need to absorb a sudden compressive force and then spring back to its original shape, compress less and less as a force increases, or deliberately fail when compression exceeds a certain point. “At the Laboratory, we often need designs for systems that undergo large deformations,” explains Sharpe. “We need to know how they will respond in nonlinear situations.” Examples in everyday life include a bicycle helmet that fractures as designed during a violent impact, and a car bumper that returns to its original

shape when lightly tapped but crumples extensively in a high-speed accident.

“It is difficult for a classically trained engineer to conceptualize all the possible shapes that solve a problem, especially radically new designs,” observes White. As an example of the potential design burden, additive manufacturing permits the placement of a different material at every corner of a repeating microtruss, which itself can vary in size, degree of stiffness, and other structural properties. As a result, the number of possible design options quickly approaches infinity, making any trial-and-error process to produce an optimized object a daunting proposition.

White states that LiDO can liberate engineers from trial and error and the overwhelming design choices afforded by additive manufacturing. Currently, an engineer uses various software packages to create a prototype design and subsequently simulates the desired output, such as calculated mass and the stress and strain such a shape would likely experience. The engineer then determines whether the design meets the prescribed specifications. If not,

the process is repeated with a revised design. LiDO reverses the process: An engineer compiles a list of desired mass and maximum stress and strain levels, after which LiDO determines the final shape and internal microstructure. Letting HPC do the hard work saves weeks of development time.

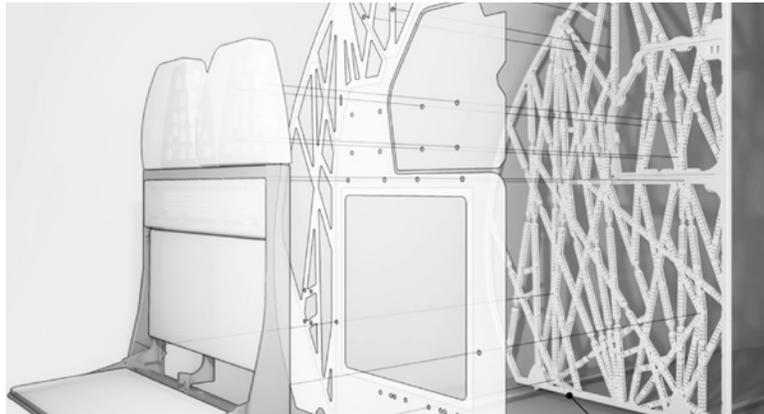
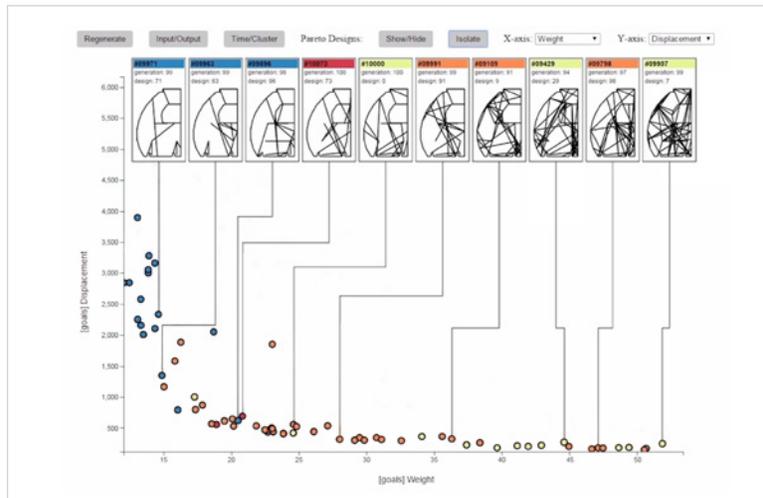
Leveraging Current Software

LiDO is massively parallel, meaning the software is designed to run on a supercomputer that uses a large number of processors simultaneously. In fact, LiDO builds upon existing software developed by Livermore’s Computation Directorate for solving huge physics problems on large parallel supercomputers such as the Laboratory’s Sequoia supercomputer, which is capable of speeds of up to 20 petaflops (one quadrillion floating-point operations per second). LiDO uses a software resource called MFEM (Modular Finite Element Methods), a Livermore-developed open-source, scalable software library for converting real-world physics problems into discrete computational representations based on finite

elements—meshes of squares, cubes, triangles, or tetrahedrons—and solving the resulting simultaneous equations, which number in the hundreds of millions. LiDO also leverages Livermore’s HYPRE library of linear solvers to enable larger, more detailed scientific simulations by solving problems more quickly than traditional methods can. HYPRE has been used by research institutions and private companies to simulate phenomena such as groundwater flow, magnetic fusion energy plasmas, blood flow through the heart, and pumping activity in oil reservoirs.

Tortorelli explains that commercially available design optimization software is limited primarily to simple physics and assumptions of linear and static behavior. Because of the small customer base, software vendors are not motivated to incorporate the complex, nonlinear physics that Livermore researchers must consider in their design problems. Academic researchers may tackle more complex design optimization problems than industry does, but few universities have at their disposal the immense supercomputer facilities needed to run integrated design optimization software.

LiDO is not expected to be finished until 2019, but researchers are already demonstrating many of its design capabilities. One emphasis is demonstrating new designs for strong, lightweight structures that require reinforcement at high-stress spots. “Such design freedom is not available with commercial software,” says White. “With LiDO, we do not have to make a part uniform. We can tailor the material architecture to accommodate varying stress levels.” White notes that historically, more than 99 percent of all design optimization problems involve maximizing stiffness, and so LiDO developers are focusing on demonstrating efficient and original designs for structures such as bridges and drones. Their design solutions involve spatially varying microarchitected



Livermore industrial partner Autodesk, Inc., has used design optimization capabilities to design a partition panel for commercial passenger jets. (top) The software’s user interface presents multiple options. (middle) The design chosen is shown integrated into existing structures. (bottom) The three-dimensionally printed metal partition panel is half as light yet just as strong, saving fuel and reducing carbon dioxide emissions.

lattices based on repeating unit cells for reduced weight and increased strength. For example, a simulated bridge that first appears to be a solid object is actually a series of repeating microtrusses, which vary in size and distribution to maximize the strength-to-weight ratio—that is, to effectively carry the load in high-stress regions but save weight in low-stress regions. This “lattice of

lattices” approach is similar to that employed in the Eiffel Tower, a structure that was considered revolutionary for its novel design when built.

Many real-world design problems faced by Livermore researchers involve multiphysics, such as a part that must withstand both thermal and mechanical loads or be able to both reduce aerodynamic drag and absorb

energy in an impact. LiDO’s multiphysics capabilities can be seen in the design of structural electromagnetic devices such as antennas that satisfy strength and stiffness requirements while only minimally attenuating electromagnetic waves. Optimized design variations for these devices feature silicon dioxide pillars composed of microlattices (for strength) topped with nanoantennas having tunable

Advancing Additive Manufacturing

For nearly a decade, Lawrence Livermore has been advancing the science of additive manufacturing. Also called three-dimensional (3D) printing, additive manufacturing uses a digital file to build 3D structures. Most additive manufacturing processes build up layers of material to precisely create objects with complex shapes engineered to handle a variety of forces. One well-established technique is direct ink writing, which deposits an ink made of silicone or other materials onto a substrate one layer at a time in a predetermined pattern. The resulting structure is then cured with heat or ultraviolet light.

By sequentially layering materials, additive manufacturing affords the ability to control both material composition and structure at multiple length scales and create objects with desirable material properties and performance. The process is being adopted by many industries to drastically reduce product development and production, particularly for low-volume specialty parts and tooling. Contrary to what the name might imply, the process actually requires less material than subtractive fabrication methods, such as machining or etching.

More than 100 material scientists, chemists, physicists, engineers, and computational scientists at Lawrence Livermore are participating in this effort to develop advanced materials and manufacturing processes. Examples include catalyst-filled beads to capture carbon dioxide from flue gas and new armor material for U.S. soldiers. Much of the effort is funded by the National Nuclear Security Administration (NNSA) in a multiyear program that is exploring and adapting the most promising technologies. The goal is to demonstrate the ability to produce complex parts with geometries that are unobtainable with conventional manufacturing methods, and with significantly less performance uncertainty.

Additive manufacturing is proving particularly valuable for stockpile stewardship, the NNSA program to ensure the continued safety, security, and effectiveness of the U.S. nuclear arsenal. The technique is helping to shrink the program’s manufacturing footprint and bring about more agile operations. Livermore researchers are also showing how additive manufacturing can improve both speed and quality in developing replacement parts, prototypes, test objects, and related materials. (See *S&TR*, January/February 2015, pp. 4–11.)

Materials scientist Chris Spadaccini, director of Livermore’s Additive Manufacturing Initiative, notes that of the dozen or so different additive manufacturing processes in use at the Laboratory, many were invented or improved upon by Livermore researchers. One example is digital holography, which reconstructs 3D geometrical information. The process was developed with researchers from the University of California at Berkeley and uses a diffractive optical element to phase-modulate a laser beam so that multiple images of a holographically shaped light field intersect in a volume of resin. Millimeter-scale parts with approximately 100-micrometer resolution form in about 10 seconds without requiring a support structure. (See the article beginning on p. 12.)

Novel products with remarkable properties continue to be achieved by Livermore researchers. In late 2017, a team announced the 3D printing of composite silicone materials that are flexible and stretchable and possess shape memory behavior. The combination of 3D printing with shape memory characteristics is often referred to as four-dimensional printing, with the fourth dimension being time. The breakthrough could lead to innovations ranging from body heat-activated helmet cushions to form-fitting shoes. Also in late 2017, Livermore researchers and collaborators at Ames National Laboratory, Georgia Tech University, and Oregon State University 3D-printed a marine-grade stainless steel, achieving unparalleled strength and high ductility. The team plans to investigate producing high-performance steels and other lighter weight alloys.

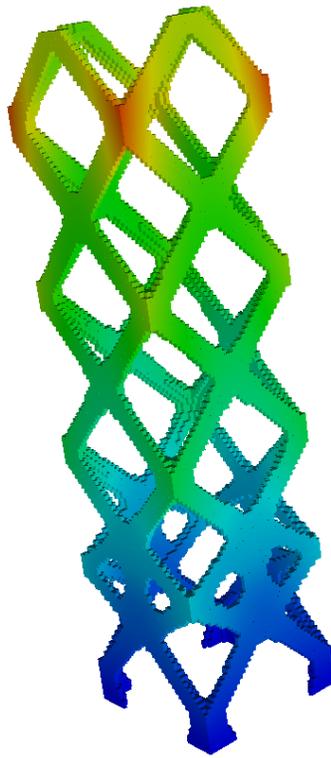
The resounding success of Livermore’s additive manufacturing capabilities, along with increasing interest expressed by U.S. industry, spurred construction of the Advanced Manufacturing Laboratory (AML), a \$10 million, 1,300-square-meter facility scheduled to open in early 2018. Located in the Livermore Valley Open Campus, AML is intended to foster partnerships between Livermore additive manufacturing experts and U.S. businesses. The facility houses the most advanced equipment in the field, including manufacturing, material evaluation, and characterization devices, along with high-performance computational modeling and simulation systems.

electromagnetic characteristics. These metamaterials can be engineered to be transparent to electromagnetic waves, to disregard only certain frequencies, or to be 100 percent reflective like a mirror.

Some shapes suggested by LiDO evoke curvatures and complex microstructural designs that are found in nature but which would be prohibitively difficult or expensive to fabricate with conventional manufacturing. These new shapes—called biomimetic—can resemble those found in living organisms. Sharpe points to mollusks whose shells have developed prodigious resistance to the attacks of predators. A cross section of such a shell resembles a brick wall with a staggered lattice architecture combined with pliable mortar. Another example is a species of shrimp that wields spines like tiny battering rams, with tremendous strength for their size.

Recognizing the Potential

Livermore's efforts are supported by the Defense Advanced Research Projects Agency (DARPA), which develops technologies for the Department of Defense and is looking to change the way the military models, designs, and manufactures its next-generation vehicles and weaponry. The agency's Transformative Design (TRADES) program funds development of algorithms that can take full advantage of new materials and fabrication methods. Jan Vandenbrande, DARPA program manager, explains, "The structural and functional complexities introduced by today's advanced materials and manufacturing methods have exceeded our capacity to simultaneously optimize all the variables involved. We have reached the fundamental limits of what our computer-aided design tools and processes can handle, and we need revolutionary new tools that can take requirements from a human designer and propose radically new concepts, shapes, and structures that would likely never be conceived by even our best



An optimized design for a column that resists twisting is shown. Red represents the highest strain, blue the lowest.

design programs today, much less by a human alone."

In January 2017, DARPA awarded a four-year, multimillion-dollar TRADES grant to Lawrence Livermore, Autodesk, the University of California at Berkeley, and the University of Texas to develop advanced tools for not only generating designs with additive manufacturing but also for better managing the complexity of those design processes. Under the project, the Laboratory is developing algorithms capable of optimizing large, complex systems and working with Autodesk to create a user-friendly graphical interface. The ultimate goal is to help the Department of Defense design game-changing systems.

Tortorelli believes that LiDO will allow the tremendous potential of additive manufacturing to finally be realized. "We

want to rethink and revolutionize design so that engineers have a clean design slate." He emphasizes that the software development effort is not aimed at taking engineers out of the design loop. Instead, he states, "We want to simplify their work and eliminate drudgery." Tortorelli expects the new design optimization paradigm to accelerate discovery and innovation, including the invention of new materials, objects, and systems with applications in the National Nuclear Security Administration's Stockpile Stewardship Program, energetic materials for defense uses, and high-energy-density target materials for fusion energy research at Livermore's National Ignition Facility. The effort will also likely inspire industry to more readily consider incorporating HPC to advance its own product development with additive manufacturing, thus advancing U.S. manufacturing as a whole.

Sharpe believes that LiDO is only an important first step in totally reinventing design. He sees another looming and intriguing aspect to the design process—incorporating aesthetics. He says, "Design is one of the frontiers of science and technology. It would be a travesty to use the same old designs with revolutionary new manufacturing technologies. Instead, we want to take full advantage of these new design capabilities, too."

—Arnie Heller

Key Words: additive manufacturing, Advanced Manufacturing Laboratory (AML), Advanced Materials and Manufacturing Initiative, Center for Design Optimization, Defense Advanced Research Projects Agency (DARPA), direct ink writing (DIW), four-dimensional printing, high-performance computing (HPC), HYPRE, Laboratory Directed Research and Development Program, Livermore Design Optimization (LiDO) software, MFEM (Modular Finite Element Methods), stockpile stewardship, three-dimensional (3D) printing, Transformative Design (TRADES) program.

For further information contact Dan Tortorelli (925) 423-5313 (tortorelli2@llnl.gov).

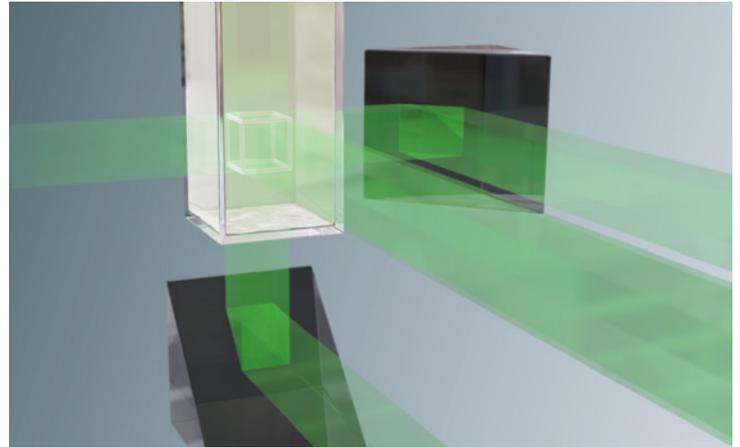
“Beaming” Objects with Volumetric Lithography

Brett Kelly, a University of California at Berkeley graduate student and Livermore collaborator, oversees the volumetric printing of an object by computed axial lithography. (Photo by Randy Wong.)

SET hundreds of years in the future, *Star Trek* depicts crew members wielding flip-to-open communicators to make surface-to-ship calls and using a replicator to instantly materialize food or spare parts. In the real-life present, smartphones have already outpaced those fictional communicators in many ways, and now we are on the verge of achieving another final-frontier technology, one capable of creating three-dimensional (3D) objects all at once rather than one piece at a time.

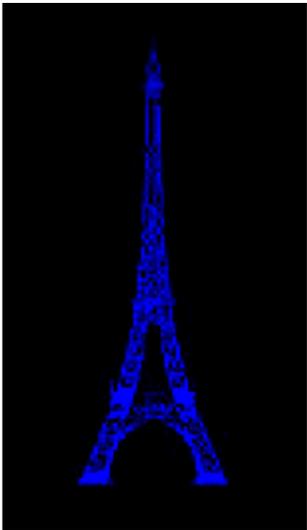
Researchers at Lawrence Livermore, in collaboration with the Massachusetts Institute of Technology, the University of California (UC) at Berkeley, and the University of Rochester, have invented two methods of volumetric lithography—using light beams to fabricate complex 3D polymer structures in one go instead of building them gradually. Livermore microtechnology engineer Maxim Shusteff says, “We wanted to explore how to make a 3D part all at once, and we decided that the easiest way would be to use light and some transparent medium. Immediately 3D holograms came to mind. Could we generate a hologram in a photosensitive material, so that the hologram cures into a physical object?” With the Laboratory’s holographic and computed axial lithography technologies—both developed with support from the Laboratory Directed Research and Development (LDRD) Program—the answer appears to be yes.

These new processes are set to energize the realm of additive manufacturing—also known as 3D printing—by combining it with lithography, which is already widely used to make microchips using photosensitive materials. In traditional 3D printing, parts are constructed layer by layer using a point source, such as a nozzle or a focused laser beam that moves back and forth across a surface to deposit or melt material in a desired pattern. In such printing



A simulation depicts holographic lithography, which begins by creating a three-dimensional (3D) hologram of the object to fabricate. A laser beam is patterned by a spatial light modulator and split into three image projection beams (green), each representing a different view of the object. Prism mirrors direct beams into a chamber containing light-sensitive resin. The resin cures wherever the three beams intersect, forming the object.

approaches, an entire two-dimensional (2D) layer may be patterned all at once. However, these techniques all have drawbacks. Shusteff explains, “The layer-by-layer approach is slow. For example, if your part has a hundred layers and each layer takes a minute to print, then the part takes almost two hours to complete. In addition, the resulting parts can have zigzagging edges. This roughness is almost always undesirable. Furthermore, unsupported structures or



Using computed axial lithography, a 3D model of the Eiffel Tower is formed. (left) Each video frame shows the shape from a slightly different perspective. (middle) Inside a rotating chamber, the beam reacts with light-sensitive resin, which begins to harden. (right) After about 2 minutes of exposure, the resin solidifies into the 3D part.

disconnected islands of material that will later connect to another layer by an overhang or a span cannot be formed layer by layer. Our new approach of creating objects in 3D all at once overcomes these limitations.”

Holographic Lithography

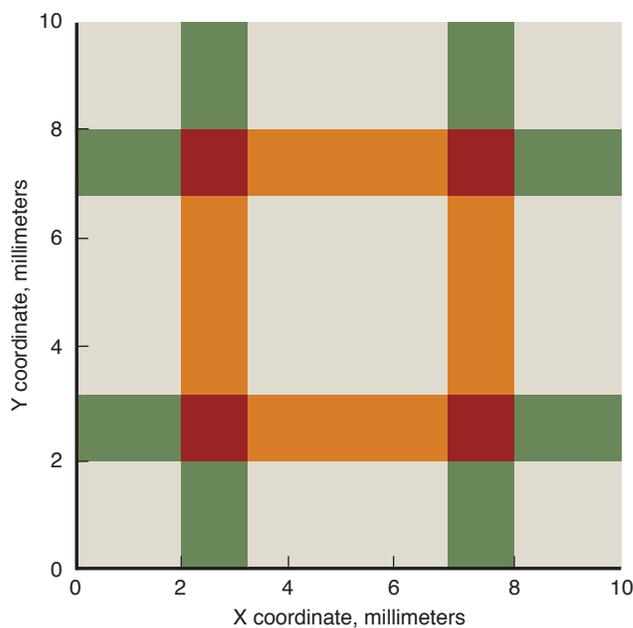
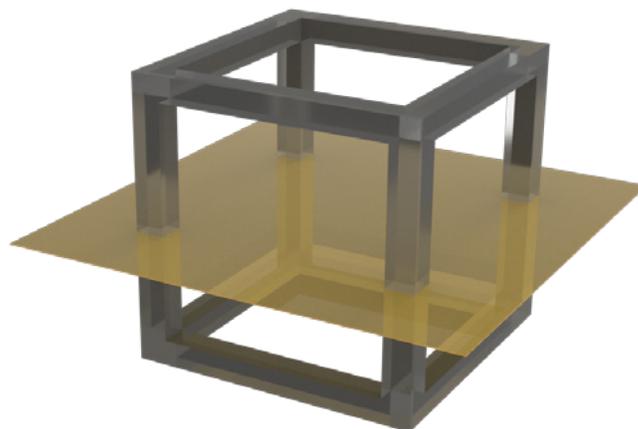
In holographic lithography, the first step is to generate a hologram of the object. Next, the hologram is broken down into three projections each representing a different orthogonal view, usually front-to-back, right-to-left, and top-to-bottom. A diode laser generates a 532-nanometer primary beam with a power of 5 to 50 milliwatts, and the beam is widened by passing through an array of optical components. After striking a spatial light modulator—an array of liquid crystal pixels on a silicon surface—the beam is patterned into the three projections spaced apart from each other inside the beam and which together comprise the single 3D image.

Refined by additional optics, the projected image overlaps two prism mirrors and a glass chamber, which contains a resin made of a photopolymer—polyethylene glycol diacrylate—with a small amount of photoinitiator. Two of the three composite image segments are directed by the mirrors into the chamber at right angles while the third projection shines head-on into the chamber. As these beams perpendicularly intersect in the chamber, the free-floating 3D structure forms in the resin as its photopolymer absorbs the light energy. A single exposure lasts only 1 to 20 seconds. Objects up to a few millimeters in size have already been successfully fabricated.

Superposition and Materialization

The absorption of light energy by the photoinitiator causes free-radical polymerization, a chemical reaction in which photopolymer molecules grow and link together. As the molecules interconnect by crosslinking, the material first achieves a gelatinous state and then finally cures into a 3D solid. In the case of a cubic lattice, for example, each projection beam has a cross-sectional shape like a square with thick sides and passes through the entire volume of resin like a square cylinder. Overlapping of the separate projections is called superposition, and at these spots the light is two to three times stronger than that of a single projection beam. The greater the intensity of light, the faster the curing occurs. Where all three projection beams converge to produce the maximum amount of light energy is where the object forms as the light energy exceeds the photopolymer’s dose threshold and crosslinking occurs. If three-beam superposition does not occur, the resin does not fully cure because the threshold is not exceeded.

Shusteff adds, “Part of the LDRD study was to determine where exposure should occur, how long exposure should last, how much light to use, what concentration of photosensitive material can achieve the desired curing rate, and how to assess the degree of

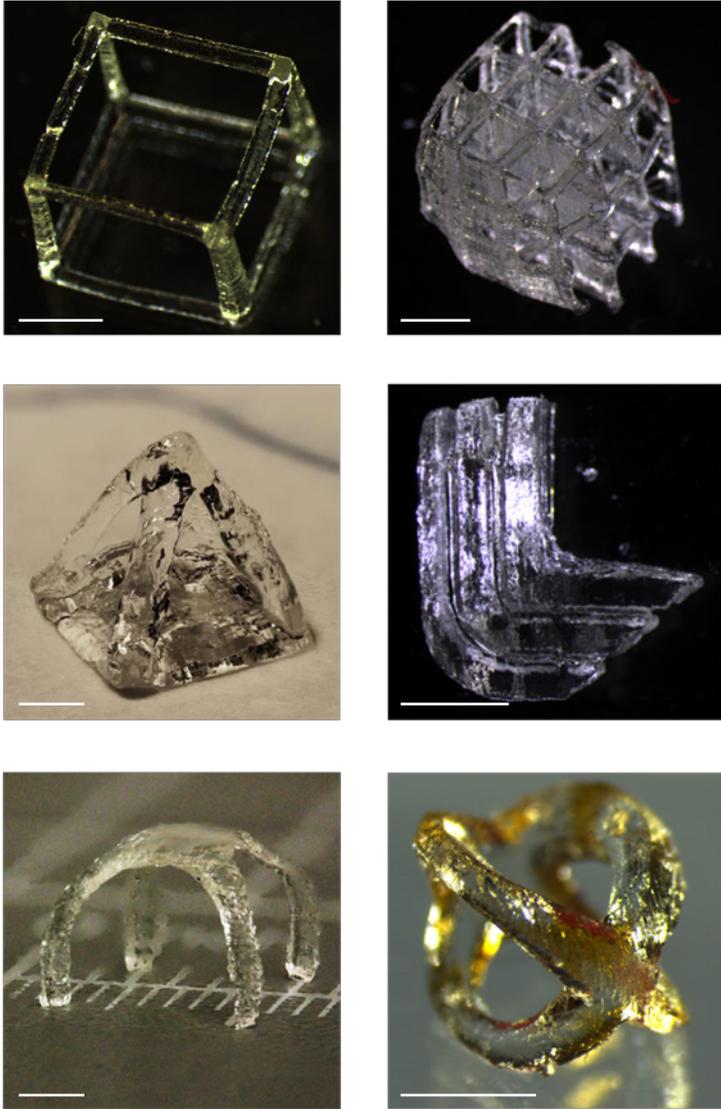


(top) A cubic lattice is shown as an example of a 3D object that can be formed by holographic lithography. The plane marks the cross section shown in the bottom image. (bottom) The relative intensity of light in the projection beams for the cross section is shown. Intensity increases with the number of beams intersecting—three beams (dark red), two beams (orange), one beam (green), and no beams (beige).

curing. In short, a timing game is played. For example, if exposure is too long, the structure overcures, and resin outside of the three-beam intersections also starts to solidify.”

Computed Axial Lithography

Forming hologram projections with a spatial light modulator is a complex, demanding process. The laser must be stringently aligned by many optical components, including multiple lenses and filters.



Photos show some of the hundreds of objects successfully fabricated with holographic lithography. The cubic lattice from the previous figure is shown in the top left. Each scale bar represents 2 millimeters.

visible light instead of x rays. Brett Kelly, a graduate student from UC Berkeley, spearheads this effort at Livermore.

In CAL, the system generates a video portraying the complete rotation of projections of the 3D object to be fabricated. Kelly explains, “Instead of using three images, we use a sequence of 1,440 images, or 4 per degree of rotation.” For roughly 1 to 3 minutes, the video images travel through a lens and into a resin chamber whose rotation rate is synchronized with the video frame rate. Each image is a different 2D pattern of light and enters the resin from a different angle. Inside the resin, the light intensity increases through superposition. Kelly adds, “By summing up all these carefully designed images, we create a distributed 3D energy dose inside the resin. With multiple rotations, the dose becomes sufficient to cure desired regions while leaving undesired regions in liquid form.” The resin used is more viscous than that in holographic lithography, but the same crosslinking process forms structures on the centimeter scale. The structures cure upon completing up to three full rotations. Because CAL uses time-multiplexed images and a weaker light source—requiring more time for the dose to exceed the photopolymer’s light energy threshold—build rates are currently slower than those of holographic lithography. However, holographic lithography’s geometric constraints are overcome.

Shusteff sees holographic lithography and CAL as complementary. “We may not always be able to fabricate a part by spinning it around in CAL or not always have access to all sides to use holographic lithography. However, the chances are we can make any structure using one technique or the other or some combination of both.” The researchers are now eagerly looking to further push the boundaries of these technologies. What other materials can be used? Can the size of a shape be scaled up and down? How can the resolution be improved? What other limitations are out there? Determined work will answer these questions. Says Shusteff, “These are certainly the directions in which we hope to take this promising technology in the future.”

—Dan Linehan

Measurements are also required to control speckle, that is, noise from the interference of coherent light. Shusteff describes another challenge: “The projection beams are basically like extrusions or collimated light and so cannot have features in the depth dimension. This characteristic imposes geometrical limitations on what structures can be made. To investigate the true limitations of geometric shapes, we developed an outgrowth project.” That investigation of possible geometries entailed asking whether the three projection beams could be aimed in other directions, not only perpendicular to one another. The team turned their attention to nonholographic projections and developed a method called computed axial lithography (CAL), which is similar to the computed tomography used in medical applications but uses

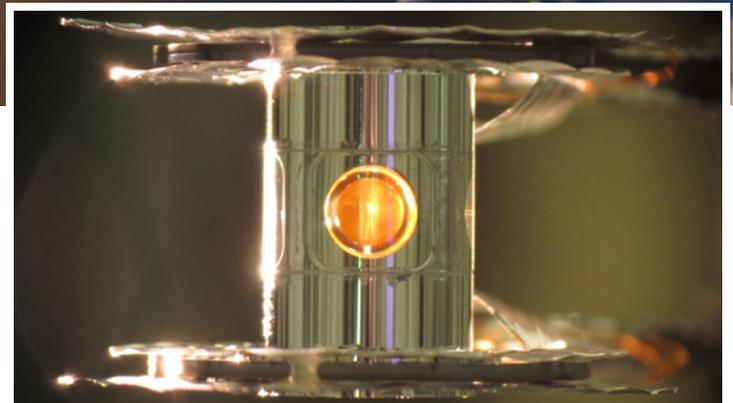
Key Words: additive manufacturing, computed axial lithography (CAL), holographic lithography, Laboratory Directed Research and Development (LDRD) Program, laser, photopolymer, spatial light modulator (SLM), superposition, three-dimensional (3D) printing, tomography.

For further information contact Maxim Shusteff (925)423-0733 (shusteff1@llnl.gov).

BIG IDEAS for Tiny Targets

FROM the 10-story-high building that could hold 3 football fields (each 48.5 meters by 109.1 meters) to the 130,000-kilogram target chamber that brings together 192 laser beams, nearly everything about Lawrence Livermore's National Ignition Facility (NIF) is gigantic—except the targets themselves. Nestled inside a cylindrical hohlraum is a spherical capsule only 2 millimeters in diameter. For inertial confinement fusion (ICF) experiments, the capsule contains a fragile, volatile mix of deuterium–tritium fuel. This sphere must rest securely in its berth until the laser beams converge inside the hohlraum and the capsule implodes, becoming the “star” of the experiment. (See *S&TR*, January/February 2016, pp. 4–11.)

Research and development efforts focused on designing, simulating, constructing, and testing NIF targets include a



(top) A Livermore scientist tests the tensile strength of carbon nanotube yarn used to support target capsules for experiments at the National Ignition Facility. (Photo by Jason Laurea.) (bottom) A target capsule, only 2 millimeters in diameter, is visible through a port in a hohlraum. (Photo by Eduard Dewald.)

multidisciplinary team responsible for one of the smallest and most important pieces of the target assembly—the material supporting the capsule inside the hohlraum. As group leader for target fabrication science and technology, Michael Stadermann describes this work as a multipronged challenge. “Supporting the capsule is a materials problem, an engineering problem, and a physics problem,” he says. “How do we make a material strong enough to withstand fabrication, handling, storage, and positioning, yet weak enough that the material doesn’t influence the fusion reaction? A successful capsule mount must provide sufficient support without interfering with the experiment.”

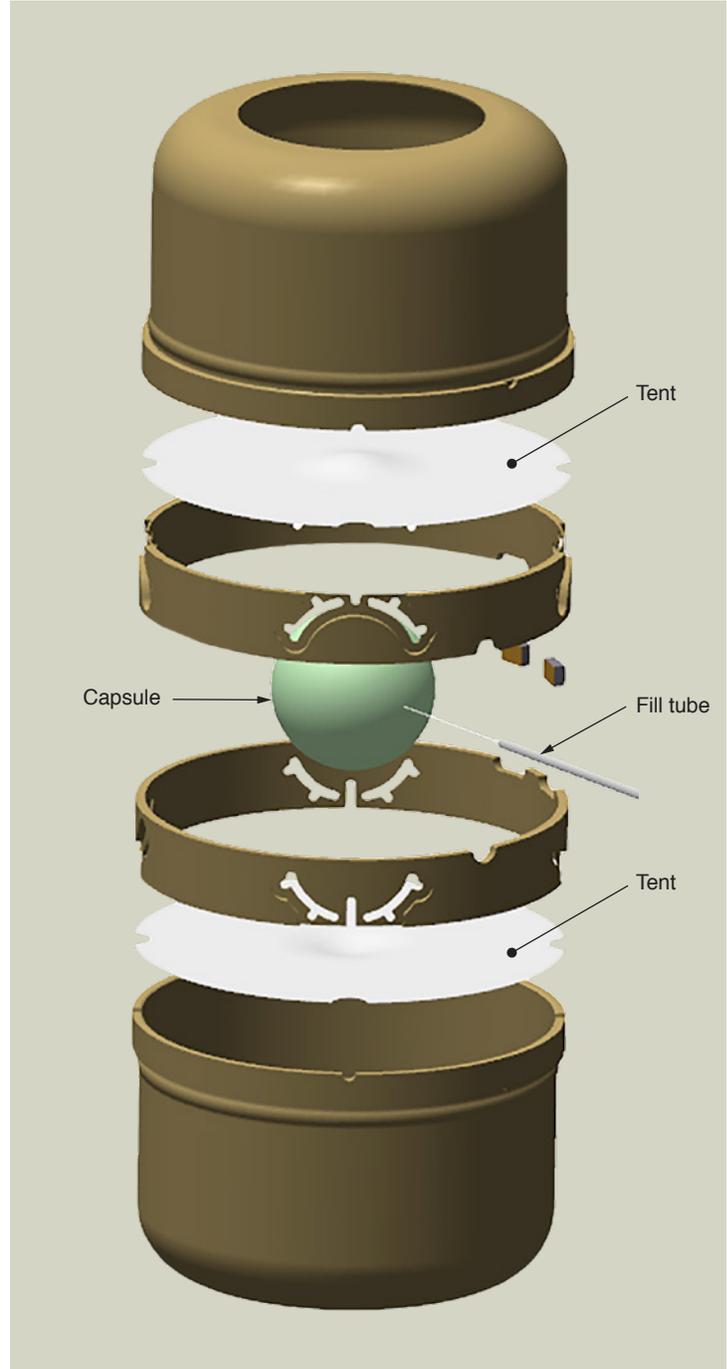
Stadermann underscores the collaborative effort necessary for fielding new target components. He notes, “All difficult problems at NIF need a dedicated team to solve them.” Physicist Vladimir Smalyuk adds, “ICF is a complicated process. To achieve ignition, we need to understand how all features in the target affect implosion, then mitigate those effects if needed. It is a team effort from beginning to end.” Through careful coordination with specialists at each phase of development, advancements in capsule support technologies are as much about the process as the product.

From Sketch Pad to Target Chamber

A capsule support design usually begins as a drawing accompanied by physics calculations. Designers, engineers, and target fabricators weigh in as Smalyuk and other NIF experimentalists develop experimental platforms to define the test parameters, such as which data to measure and which diagnostic techniques to use. Stadermann says, “Deciding which concepts to pursue is a challenge.” Not every idea outlives the sketch pad, and no detail is too small for consideration. Changing even a single variable could have multiple effects on implosion, so the team uses computer simulations to predict a design’s performance. Smalyuk emphasizes the importance of focused experiments to complement computational results. He says, “Every experiment reveals something you did not expect.”

Once initially approved, a design then undergoes rigorous evaluation. A series of target fabrication tests is conducted, including materials testing to measure specific properties and determine feasibility, assembly testing to check for centering and static stability, dynamic testing for vibration and other factors, and cryogenic layering tests using Livermore’s Integrated Target Proofing System. Stadermann notes, “We have to demonstrate that the device can survive assembly before going any further. A design passes through many hands before proving its value.” A prototype that performs well in this stage moves on to the NIF target chamber, where shots are conducted to measure perturbations and implosion efficiency. Data produced by these shots are used to validate and augment simulation codes.

NIF experimental designs need time to mature. Simple capsule support designs can be ready for the target chamber in less than



A rendering shows a design for target support that splits the hohlraum into four segments to minimize contact between the tents and capsule. Each tent is secured at its edge by two segments. Notches and holes in the hohlraum accommodate other aspects of target assembly and placement, such as a port for the capsule’s fill tube. One risk of this design is energy leakage through the ports or seams between two hohlraum segments.

a year, whereas more complicated designs may require two or more years of preparation. Iterations can take another six months of development, even if only a minor modification is made, such as repositioning a piece by a few micrometers. “Each iteration increases our understanding of ICF,” says Smalyuk. “Nature is always more complex than our imagination.”

Supporting Something with Nothing

A decade ago, thin polymer tents provided an early solution to the problem of capsule support. In this setup, two membranes are attached to the walls of the hohlraum, one above the other, with the capsule suspended between them. The membranes are bent into tented shapes around the capsule’s peaks. Over time, NIF researchers realized that the tents caused pressure and density asymmetries, decreasing implosion efficiency. Smalyuk says, “Tents produced surprisingly large modulations.” Using x-ray radiography, scientists determined that these perturbations increased with tent thickness. However, thinner tents also had limitations—because of confinement, a film’s mechanical properties changed as its thinness approached a single layer of the molecules. These changes both led to film failure after target assembly and were predicted to offset the benefits of reduced thickness, so Stadermann and colleagues began exploring alternate approaches.

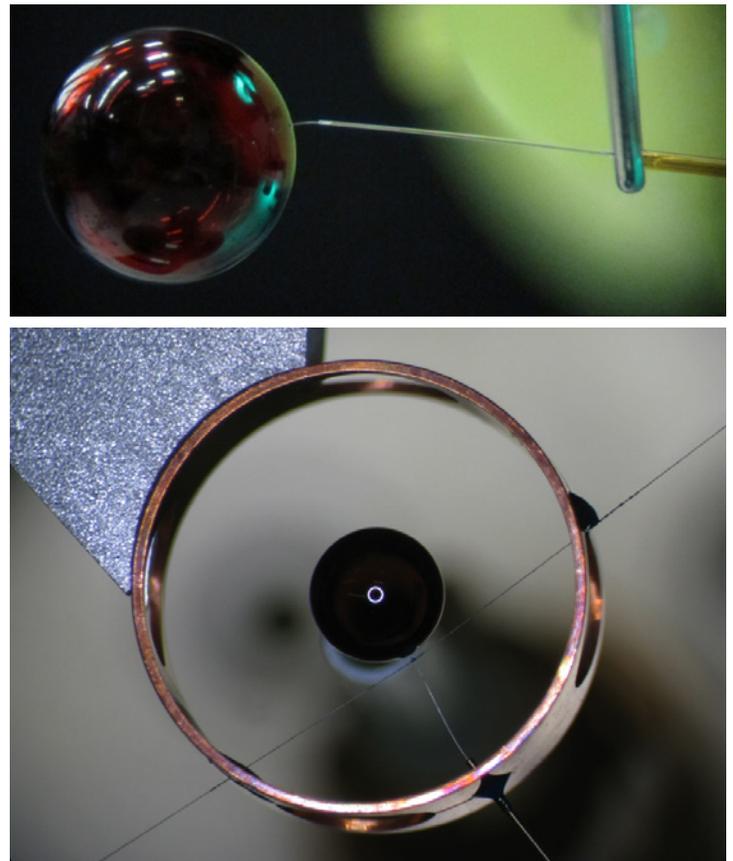
By 2014, the team had come up with dozens of ideas involving a variety of materials and attachment techniques. Stadermann explains, “From there, we evolved our process to find common denominators and eliminate duplicates.” A major problem to solve with any target-supporting approach is reducing the amount of supporting material touching the capsule, thereby decreasing perturbation. Stadermann explains, “How can we support the capsule with as little material as possible? To put it more simply, how do we hold something with nothing? Making a material thinner or exposing it to cryogenic temperatures changes its mechanical properties. Designs that initially show potential can be eliminated because of this change.” Three solutions have come far in recent testing—a four-part hohlraum with polar tents, a supported fill tube, and the tetra cage.

Promising Approaches

Despite earlier outcomes, the team decided to continue exploring tents. The idea of sandwiching the capsule between two tents to reduce surface contact led to the four-part hohlraum, in which the walls of a hohlraum segmented into four parts clamp

the tents’ edges. With a stabilized perimeter, the membranes touch only the capsule’s poles. Stadermann acknowledges the miniscule margins of error that come with fine-tuning the four-part design. He says, “When we reduce the amount of deflection, or bend, in the tents, the tents must be stiffened to have sufficient force for holding the capsule. However, if made too stiff, the tents can break during assembly.” This tradeoff, combined with the added task of stocking more hohlraum parts, is proving worthwhile. Data from multiple shots conducted at NIF show improvement over the original two-tent design, and the four-part hohlraum is now part of standard target production.

For another method of capsule support, the team looked more closely at the 10-micrometer-diameter glass tube that fills the capsule with fuel. A conventional fill tube is too flimsy to hold the capsule in place without drooping and causing vibrations. Furthermore, the capsule’s weight stresses its bond with the fill tube. Consequently, Stadermann’s team attached a rod to the hohlraum walls, running it perpendicular to the fill tube, with the tube resting on top. Testing revealed an issue with the cantilevered design: The closer the rod is to the capsule end of the fill tube, the more the rod affects implosion. In a modified concept called a “fishing pole,” the



Livermore researchers are also exploring enhancements to an existing device used in target assembly, instead of supporting the capsule itself. (top) One approach involves creating a fill tube with a thicker diameter for all but 200 micrometers of its length. (bottom) Another method of supporting the fill tube includes a perpendicular cross-piece.

(top) Carbon nanotubes are produced in a densely packed forest. Individual strands are separated and pulled together into a wedge shape, then twisted into a yarn. (bottom) Four yarns make up the tetra cage formation, with the capsule suspended between two pairs.

team expanded the fill tube to a thickness of 30 micrometers over most of its length, returning to the 10-micrometer diameter just short of the capsule's surface. Again, the team discovered an unexpected effect. Smalyuk explains, "The fill tube produced shadows on the capsule from the hohlraum x-ray drive. These shadows would interfere with x rays angling off the walls, introducing asymmetry into implosion." Therefore, these and related designs for fill tube supports continue to undergo stability modifications and hydrodynamic growth radiography testing.

A third approach to capsule support began with spider silk, an ultrathin substance known for its high density and excellent tensile strength. The team examined silk taken from live spiders caught in Stadermann's garden and specimens ordered on the Internet but found the creatures' silk to be inconsistent. The researchers therefore decided to make synthetic fibers using carbon nanotechnology. The process begins with a seeded catalyst subjected to thermal chemical vapor deposition, yielding a multiwalled "forest" of nanotubes. By twisting millions of such nanotubes together, the team generates thin, sturdy yarns that are then fortified with vapor-deposited polymers. Four yarns come together inside the hohlraum in an orthogonal configuration called a tetra cage. This innovative design supports the capsule between two pairs of carbon nanotube yarns—one pair under the capsule and one pair above. Stadermann states, "Now we are trying to shrink these yarns to less than 1 micrometer in diameter

to reduce perturbations even further."

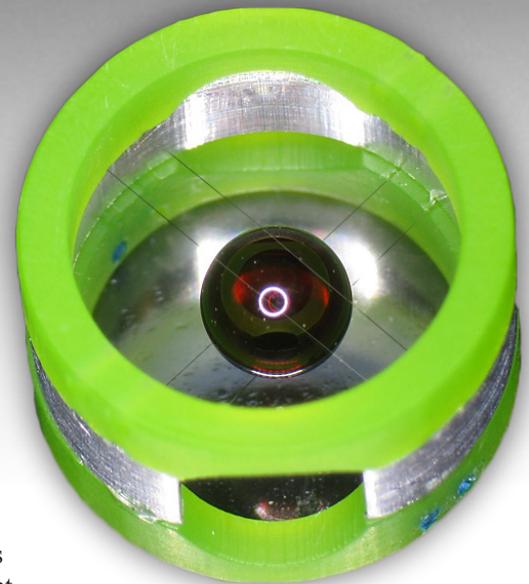
Other capsule support concepts are in development.

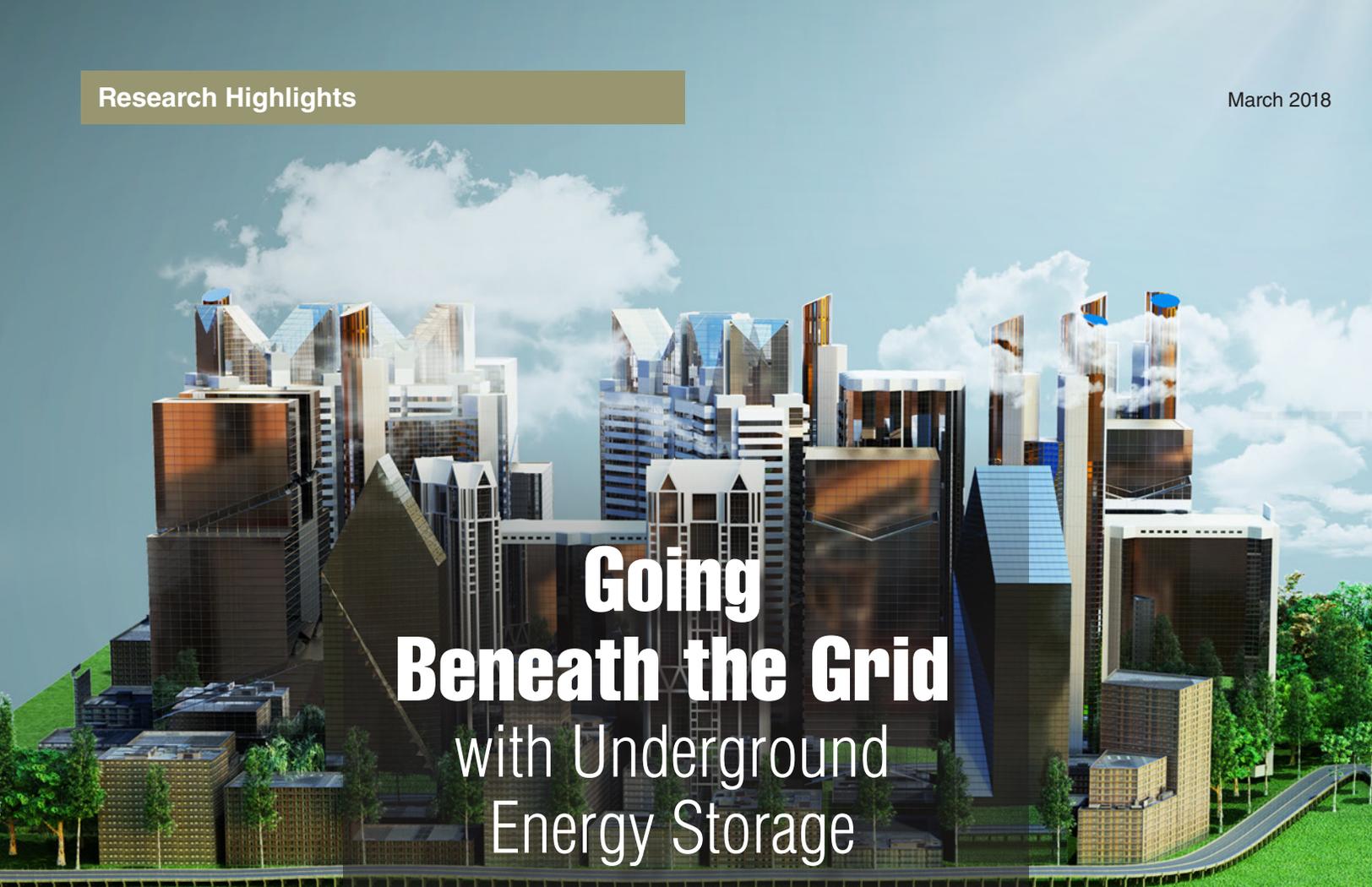
For instance, the team is working on a solution that uses magnets to levitate a capsule coated with a superconducting material, eliminating the need for a fill tube or tents. Another fill tube design positions the tube tangentially to the capsule instead of connecting perpendicularly to the surface. In another recent accomplishment, a 5-micrometer-diameter fill tube sufficiently supported the capsule while achieving the highest total neutron yield to date. Smalyuk notes, "Behind each split-second shot are years of teamwork. This neutron yield milestone was achieved because of all the hard work that came before."

—Holly Auten

Key Words: capsule, carbon nanotube, deuterium-tritium fuel, fill tube, hohlraum, implosion, inertial confinement fusion (ICF), National Ignition Facility (NIF), target science and technology, tetra cage.

For further information contact Michael Stadermann (925) 423-9128 (stadermann2@llnl.gov).





Going Beneath the Grid

with Underground
Energy Storage



SINCE 2000, the amount of clean energy generated annually in the United States has increased by almost 63 percent, while carbon dioxide (CO₂) emissions have decreased by almost 10 percent. This trend suggests a connection between the increased use of renewable energy and reduced CO₂ emissions, which is good news for the environment. However, the increase in renewable energy production has not come without problems. In general, renewable energy sources are either cyclic (as in the case of solar) or unpredictable and seasonally variable (as with wind), often resulting in a mismatch between supply and demand.

In California, renewable sources account for approximately 25 percent of the state's energy production, but the supply-and-demand mismatch means not all renewable energy generated is used. In fact, California's renewable energy production has been so high at times that the state has paid other states to take on the excess to avoid overloading its electric grid. Thus an unexpected energy crisis exists—the crisis of producing too much. The problem stems chiefly from the lack of a grid system advanced enough to keep up with increased renewable production coupled with an inability to store energy for extended periods of time.

Livermore geoscientist Tom Buscheck and retired engineer Ravi Upadhye are working on a technology with the potential to solve both of these problems and help reduce CO₂ emissions. Known as the Earth Battery, the approach uses multiple fluids to store energy as pressure and heat underground. The system includes features of compressed-air energy storage (CAES) in that compressed air can be used. However, the Earth Battery can also use compressed CO₂ along with pressurized, heated brine to store and discharge clean energy.

Innovating Compressed-Air Energy Storage

The idea of storing compressed air underground as a renewable energy resource is not new. In fact, two plants in the world currently operate on this concept: the McIntosh CAES facility in Alabama and the Huntorf CAES Power Plant in Germany. Such conventional CAES systems take advantage of lower cost energy during off-peak demand hours to support energy generation during peak hours. During periods of low energy demand, electricity is used to compress air in several stages. The air is cooled after each stage to facilitate efficient compression, and the excess heat is released into the atmosphere. The relatively cool, compressed air is then pumped into an underground salt cavern for storage. During peak energy demand hours, the stored air is released into a piping system and mixed with natural gas for combustion in expanders, which rotate a generator to produce electricity. Conventional CAES successfully stores energy for later use, but limitations include wasting most of the heat generated during compression. In addition, storage

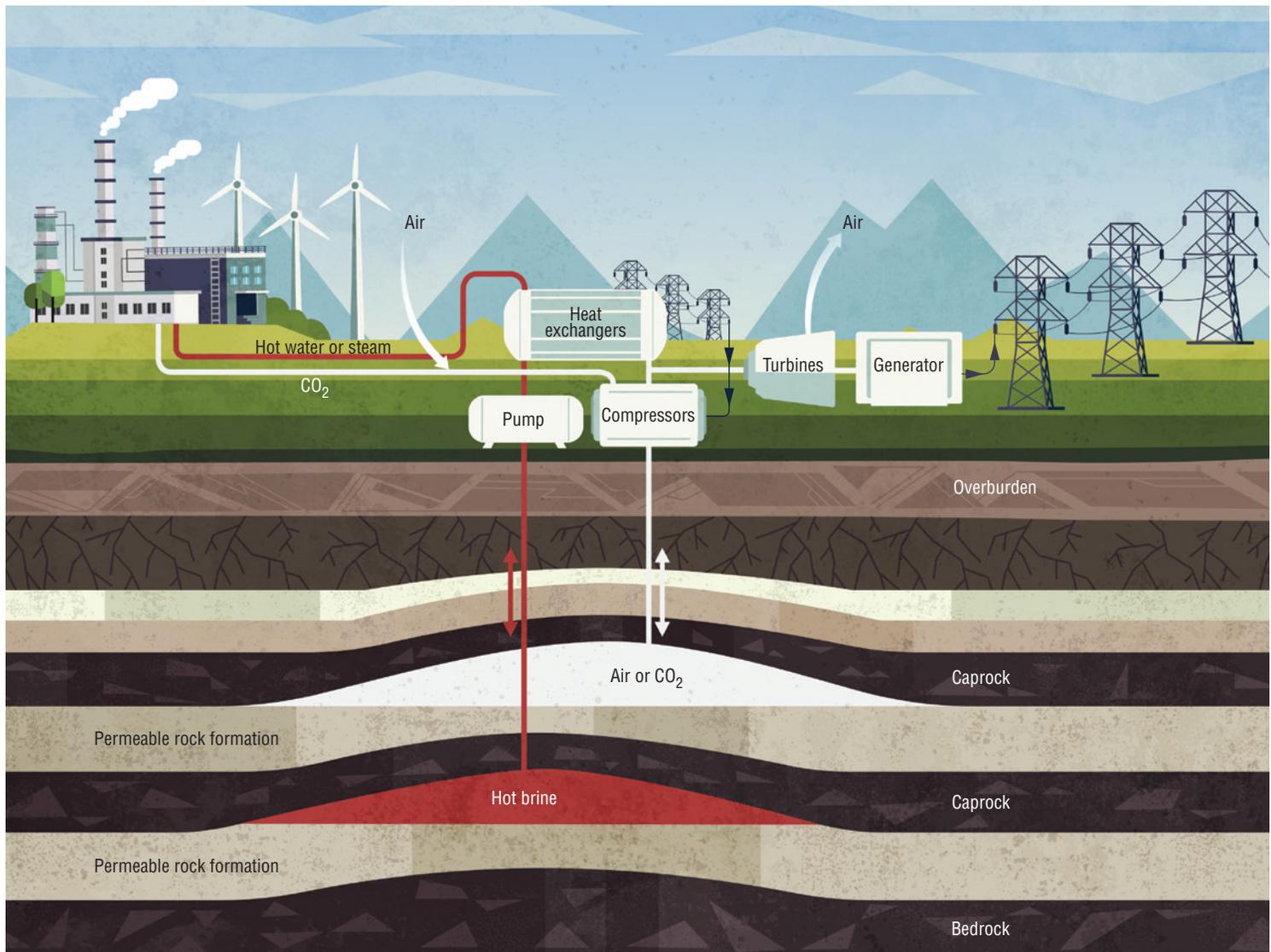


The compressed-air energy storage (CAES) facility at Alabama's McIntosh Power Plant is already using CAES in generating renewable energy. The Earth Battery would use some of the features of CAES. (Photo courtesy of PowerSouth Energy Cooperative.)

of the compressed air in salt caverns limits storage to certain geographic locations and a duration of only a few hours.

Livermore's Earth Battery concept improves upon CAES in several ways. Rather than disposing of the excess heat, the Earth Battery uses brine from an underground reservoir to cool the air after each compression stage and then stores the heat underground as hot brine. When electricity is needed, the hot brine heats the compressed air before the latter enters the expanders. This innovation eliminates the need to burn natural gas to heat the air. The Earth Battery can also store energy in porous rock, which increases storage capacity, storage times, and the range of possible sites. In addition, CO₂ can be used instead of air, making geologic CO₂ sequestration more economically viable and adding a pathway for reducing CO₂ emissions.

Buscheck says, "In the Earth Battery concept, either air or CO₂ can be used as a supplemental nonaqueous working fluid to store energy as pressure underground. We actually started with the idea of using supercritical CO₂ captured from fossil-energy power plant emissions as the working fluid." Research on the CO₂ version is a collaboration between Livermore and colleagues at the University of Minnesota, Ohio State University, and Switzerland's ETH Zürich. He adds, "The working fluid acts like a hydraulic jack to elevate the pressure and, being compressible, also functions like a shock absorber." The benefit of supercritical CO₂ lies in its dense, liquidlike



As shown in this greatly simplified illustration, the Earth Battery contains two or more compression stages and two or more expansion stages. During the charge (compression) cycle, air is compressed and cooled multiple times before being stored underground, along with hot brine. During the discharge (expansion) cycle, high-pressure cool air—or carbon dioxide (CO₂)—and hot brine from the wells are cycled through heat exchangers and expanders before the air or CO₂ is finally released into the atmosphere and the cold brine is sent back underground. The Earth Battery can also store heat from an external source, such as a base-load power plant.

state, allowing for a storage density that is 50 to 70 percent of the density of water, compared to only 10 to 30 percent when using compressed air. Supercritical CO₂ can displace the brine and create artesian (that is, overpressured) flows to wells, thus producing naturally hot geothermal brine. The displaced brine can be further heated as necessary with a clean heat source, such as excess thermal energy from a base-load power plant.

Buscheck explains, “A challenge we have today with clean base-load power, such as nuclear power plants, is that they are very expensive to build but relatively low cost to operate and thus must be operated continuously to be economically viable. These plants create heat used to generate electricity. The Earth Battery does not require constant electricity generation. Instead, some of that heat can be stored underground for later use at peak

demand times. This approach can also be combined with solar thermal energy.”

Because air is less expensive and less complicated to acquire than CO₂, the team hopes to use compressed air to test the Earth Battery concept in an initial pilot demonstration project. Air would be a good proxy for CO₂. Buscheck says, “Wherever we are able to demonstrate that air can be safely stored, storing CO₂ efficiently and safely should also be possible.”

The next step in establishing the concept was determining what type of reservoirs could be used for energy storage. Buscheck explains, “The reservoir must be a porous, permeable rock formation overlain with an impermeable caprock, so that the buoyant, pressurized fluids can move freely out of and into the wells but do not leak into shallower rock formations.” In a feasibility study funded by the Laboratory Directed Research and Development Program, the team examined two stacked reservoirs—an upper reservoir for storing air and a lower reservoir for storing hot brine. Sedimentary rock, such as sandstone or limestone, is often permeable enough to store air, CO₂, and hot brine, while shale caprocks should prevent upward leakage of the fluids. Such geologic formations—already used for CO₂ and natural gas storage—are widespread and would allow for more possible deployment sites. Because natural gas has properties similar to those of air, the team’s technology could even be used in depleted gas production fields, which are more widespread than natural gas storage sites.

From Earth to Grid

Once adequately stored, how can energy be quickly extracted from the ground when needed to produce electricity? With the Earth Battery, energy is retrieved by letting the pressurized air and hot brine flow to the power plant, which converts the stored energy to electricity. This setup differs significantly from renewable geothermal energy, which requires up to half of the generated electricity simply to retrieve the hot fluid for use by the power plant. This effort, known as the parasitic load, reduces the net power that a plant can deliver to the grid.

In contrast, the Earth Battery uses excess energy to create artesian conditions in the storage reservoirs, so operators can take advantage of time shifting—strategically planning when to impose the parasitic loads needed to create artesian conditions. With a gas turbine, about two-thirds of the power generated is used to compress air, leaving only about one-third of the gross power as electricity for the grid. With time shifting, inexpensive energy from off-peak demand hours can be used to precompress the air and generate heat so that when electricity is most needed, the majority of the gross power can be delivered to customers. This process makes more energy available when demand exceeds supply, such as on cloudy or windless days.

An advantage of using supercritical CO₂ over compressed air is the thermosiphon effect of CO₂—the reduction in CO₂

viscosity upon heating by hot underground rock, allowing CO₂ to flow more readily. Flow rates are also increased by the expansion of CO₂ as it is heated. Furthermore, the Earth Battery circulates the CO₂ in a closed loop, constantly maintaining supercritical pressures and thereby reducing the parasitic load required to reinject the CO₂ back into the reservoir. A closed loop keeps CO₂ from being released into the atmosphere, whereas the use of air allows an open loop, resulting in air being exhausted into the atmosphere.

Although using CO₂ entails a longer development horizon than using air, the former offers the dual benefits of storing energy and keeping captured CO₂ out of the Earth’s atmosphere. To enable the quick extraction of energy when needed, the team plans to use excess thermal energy to keep the heat exchangers hot, thus reducing ramp-up time when generating electricity. Says Upadhye, “It’s like taking a shower. You normally have to wait a minute or so for all the pipes to get warm, but if you already have hot water circulating, it will be available more quickly.”

Testing and Refinement

To test the effectiveness of their technology, the team has used the NUFT flow-and-transport code and Aspen Plus process-modeling software to assess the efficiency and cost of various energy storage designs for using compressed air. The researchers hope to soon launch a pilot demonstration project using a handful of air injection and production wells. Says Buscheck, “We would first field-test underground air storage and probably store the heat aboveground by more conventional means, or we might try field-testing heat and air storage in the same section of rock.”

The team factored environmental considerations into the development of their technology as well. “An environmental concern is induced seismicity, that is, earthquakes caused by increased underground pressure,” says Buscheck. He explains that ideally, the hot brine and air storage zones would be arranged in a manner that allows the air to function as a shock absorber for both fluids. “We are putting a lot of thought into reservoir pressure management to minimize the risk of seismicity. In fact, reducing seismicity was one of the first topics we examined. We want to ensure that the Earth Battery is safe in addition to being cost effective and environmentally responsible.”

—Lauren Casonhua

Key Words: carbon dioxide (CO₂), compressed-air energy storage (CAES), Earth Battery, geothermal energy, Laboratory Directed Research and Development Program, renewable energy, supercritical CO₂, underground energy storage.

For further information contact Tom Buscheck (925) 423-9390 (buscheck1@llnl.gov).

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory. For the full text of a patent, enter the seven-digit number in the search box at the U.S. Patent and Trademark Office's website (<http://www.uspto.gov>).

Patents

Modeling the Long-Term Evolution of Space Debris

Sergei Nikolaev, Willem H. De Vries, John R. Henderson, Matthew A. Horsley, Ming Jiang, JoAnne L. Levatin, Scot S. Olivier, Alexander J. Pertica, Donald W. Phillion, Harry K. Springer
U.S. Patent 9,586,704 B2
March 7, 2017

Method to Pattern <10 Micrometer Conducting and Passivating Features on 3D Substrates for Implantable Devices

Vanessa Tolosa, Satinderpall S. Pannu, Heeral Sheth, Angela C. Tooker, Kedar G. Shah, Sarah H. Felix
U.S. Patent 9,694,190 B2
July 4, 2017

Origami Enabled Manufacturing Systems and Methods

Hanqing Jiang, Hongyu Yu, Goran Konjevod, Yong Xu
U.S. Patent 9,706,646 B2
July 11, 2017

Shape Memory Polymers

Thomas S. Wilson, Jane P. Bearinger
U.S. Patent 9,745,402 B2
August 29, 2017

Resistively Heated Shape Memory Polymer Device

John E. Marion, III, Jane P. Bearinger, Thomas S. Wilson, Duncan J. Maitland
U.S. Patent 9,752,562 B2
September 5, 2017

Phased Charging and Discharging in Capacitive Desalination

Michael Stadermann, Yatian Qu, Juan G. Santiago, Ali Hemmatifar
U.S. Patent 9,758,392 B2
September 12, 2017

Awards

Laboratory physicist **Dmitri Ryutov** was awarded the **American Physical Society's James Clerk Maxwell Prize for Plasma Physics**. He was cited "for many outstanding contributions to the theoretical plasma physics of low and high energy density plasmas, open and closed magnetic configurations, and laboratory and astrophysical systems." The recognized work was conducted during Ryutov's 22-year career at Livermore and, prior to that, at Russia's Budker Institute of Nuclear Physics.

The prize, established in 1975 in honor of Scottish physicist James Clerk Maxwell, is sponsored by General Atomics and recognizes outstanding contributions to the field of plasma physics. Recipients are given \$10,000 and a certificate citing their contributions.

Ryutov recently retired from the Laboratory but continues a close connection as a visiting science professional. He is a theoretical physicist with interests in plasma physics and its applications, the environmental aspects of energy production, space and astrophysical plasmas, x-ray optics, and advanced dynamics.

The 26th **International Association for Computing Machinery Symposium on High-Performance Parallel and Distributed Computing**, one of the world's premier computer science conferences, recognized Lawrence Livermore researcher **Edgar A. Leon** and his collaborators Bo Li and Kirk Cameron from Virginia Polytechnic Institute and State University with the **Karsten Schwan Best Paper Award** for their modeling work on parallel performance.

The paper—"COS: A Parallel Performance Model for Dynamic Variations in Processor Speed, Memory Speed and Thread Concurrency"—describes an analytical model of computational performance called compute-overlap-stall (COS), which accurately captures the combined effects of dynamic variations posed by different operating modes on execution time. Understanding these effects may play a key role in helping future

high-performance systems meet the challenging demands of parallel scientific applications.

Livermore atmospheric scientist **Ben Santer** was selected as a **fellow** of the **American Meteorological Society (AMS)**. AMS fellows must have made "outstanding contributions to the atmospheric or related oceanic or hydrologic sciences or their applications during a substantial number of years." Santer's research focuses on topics such as climate model evaluation, statistical methods in climate science, and identification of natural and anthropogenic "fingerprints" in observed climate records. His early research on the climatic effects of combined changes in greenhouse gases and sulfate aerosols contributed to the historic "discernible human influence" conclusion of the 1995 report by the Intergovernmental Panel on Climate Change.

In recognition of his outstanding leadership and service to the nation, **Victor H. Reis** was named the third recipient of the **John S. Foster Jr. Medal**. Established by **Lawrence Livermore National Security, LLC**, and bestowed annually by the Laboratory director, the medal recognizes exceptional leadership in scientific, technical, and engineering development and policy formulation in support of U.S. nuclear security.

After the U.S. moratorium on nuclear testing in 1992, Reis was among the first to recognize the need for a new, formal program to maintain the U.S. nuclear stockpile with data from supercomputer simulation and multiscale experiments.

From 1993 to 1999, Reis served as assistant secretary for Defense Programs in the Department of Energy, where he developed the Stockpile Stewardship Program and its associated Accelerated Strategic Computing Initiative, now the Advanced Simulation and Computing Program.

Leading a Revolution in Design

Additive manufacturing technologies allow extreme levels of control over shape and material composition at scales down to nanometers. The rapidly growing field also creates the potential to engineer materials with desired structural, thermal, electrical, chemical, and photonic properties in a single package. Lawrence Livermore researchers are creating new materials that can only be realized using additive manufacturing. The new parts and systems, intended for Livermore's national security missions, offer greater performance, reduced time to manufacture, less waste, and often lower cost. Livermore's Center for Design Optimization was established in October 2016 in response to the critical need for a comprehensive computing environment for Laboratory engineers that takes full advantage of additive manufacturing. With funding from the Laboratory Directed Research and Development Program, the center launched a three-year Strategic Initiative in Computational Design Optimization to develop the efficient software package called Livermore Design Optimization (LiDO). With LiDO, the tremendous potential of additive manufacturing will likely be realized for the first time, and a true revolution in design will be launched.

Contact: Dan Tortorelli (925) 423-5313 (tortorelli2@llnl.gov).

30 Years of Accelerating Science



The Center for Accelerator Mass Spectrometry brings three decades of scientific and technical achievements to bear on a wide variety of Livermore programs.

Also in April/May

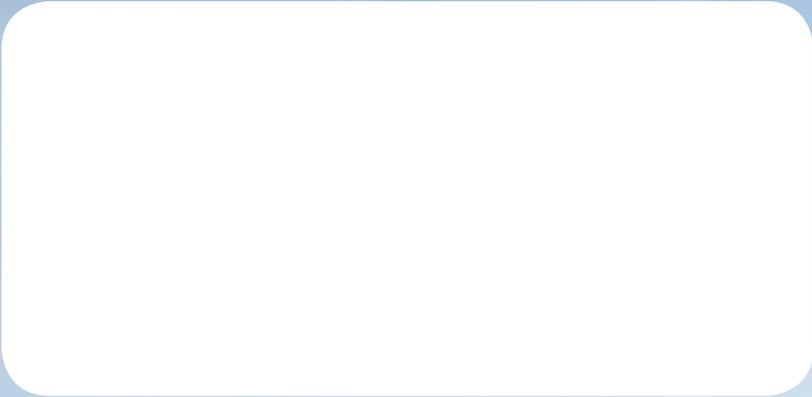
In R&D Magazine's annual competition for the top industrial inventions, Laboratory researchers won awards for the following:

- *Applied Biosystems™ Axiom™ Microbiome Array*
- *Radiation Field Training Simulator*
- *The Earth System Grid Federation*
- *Four other technologies developed with collaborators.*

At the National Ignition Facility, a new generation of x-ray diagnostics is born.

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